

Chloral

75-87-6 | DTXSID7024744

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 11.7

Global applicability domain: Inside

Local applicability domain index: 5.00e-01

Confidence level: 7.50e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,1-Dichloroethylene</div> <div>Measured: 12.9</div> <div>Predicted: 9.95</div>	<div>Image not found</div> <div>Allyl chloride</div> <div>Measured: 5.01</div> <div>Predicted: 6.46</div>	<div>Image not found</div> <div>Trichloroethylene</div> <div>Measured: 15.8</div> <div>Predicted: 15.2</div>
<div>Image not found</div> <div>Bis(2-chloroethyl) ether</div> <div>Measured: 10.0</div> <div>Predicted: 9.54</div>	<div>Image not found</div> <div>Dichloromethane</div> <div>Measured: 22.9</div> <div>Predicted: 12.6</div>	